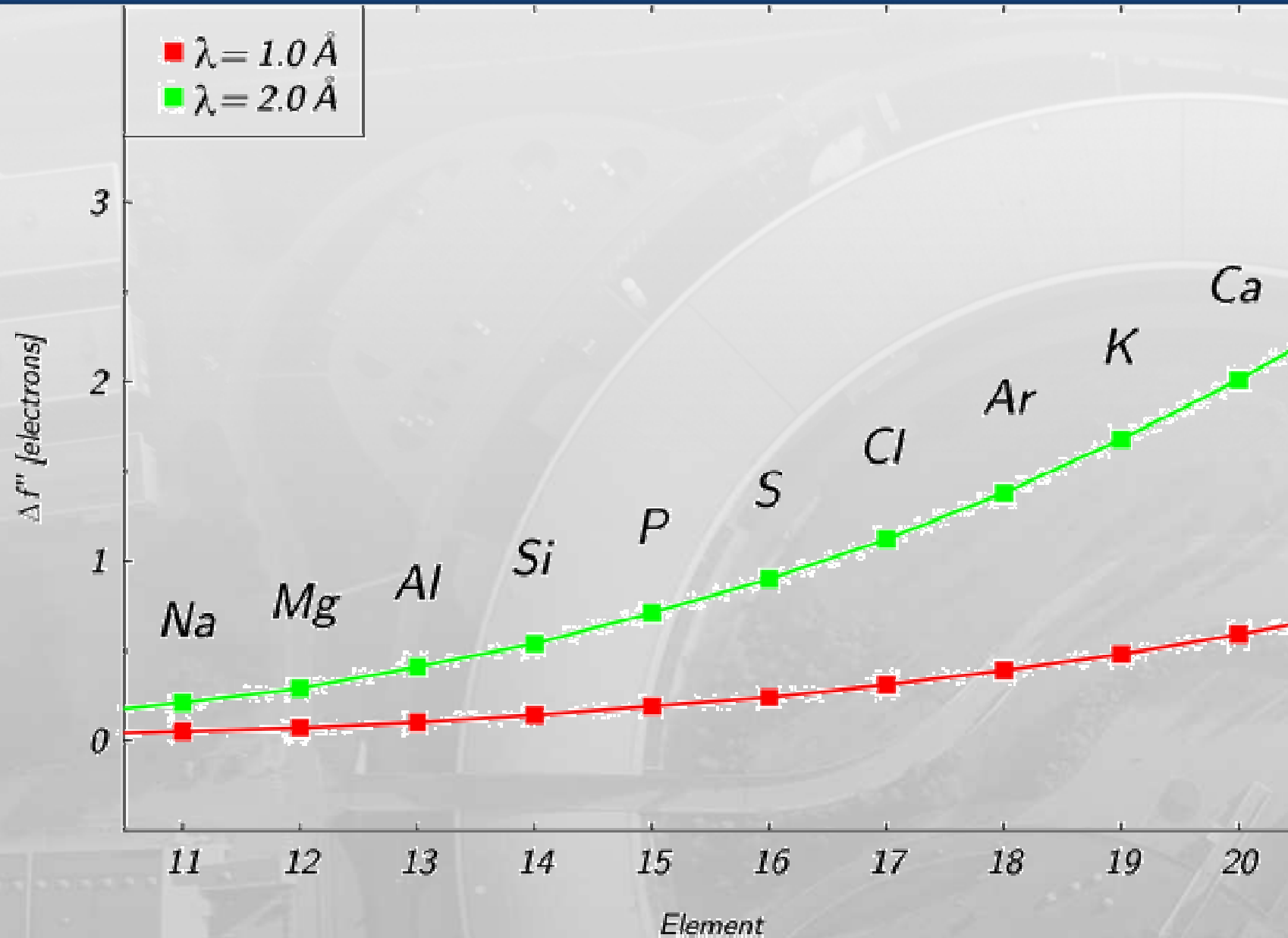


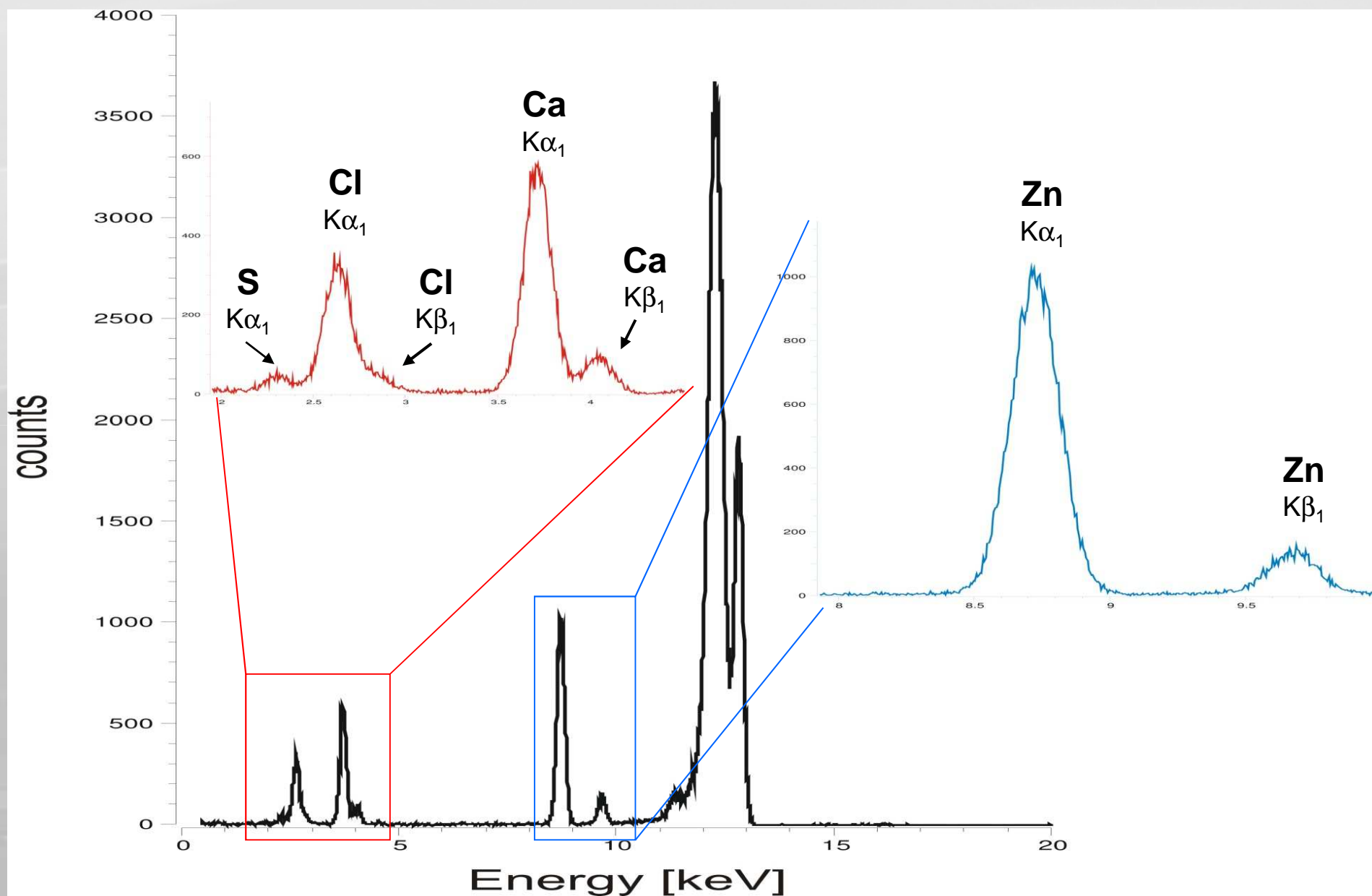
Get more information from your Structure: Careful determination of the substructure

**Christoph Mueller-Dieckmann
E.S.R.F. Grenoble, France**

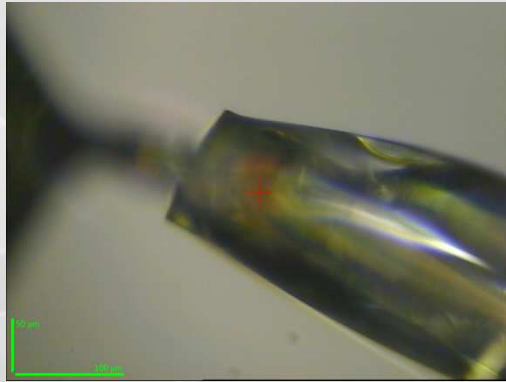
Surely, you want to have

- Best model to interpret electron density
- Additional information on biological relevant atoms (e.g. ligand binding / orientation)
- Double-check your model (position of Met/Cys)

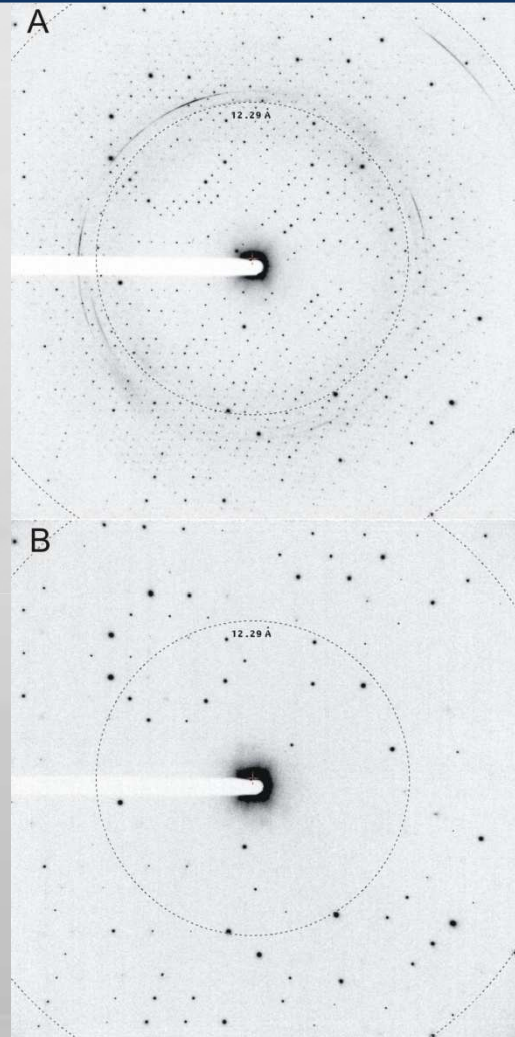




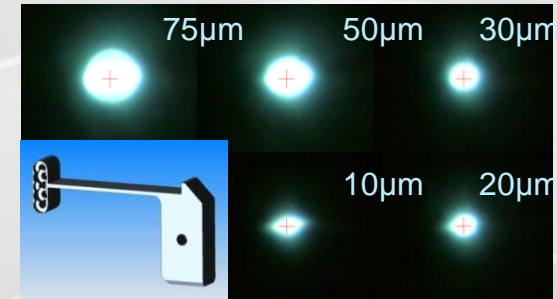
- Accurate data collection / processing



=> Use data collection strategy programme to avoid radiation damage



=> Avoid contamination



=> Match beam to crystal

Etc....

- Accurate data collection / processing
- If phasing: high redundancy / multiplicity

OMEGA

KAPPA axis

Torque limited rotation
0-270 Deg, ± 0.2 Deg

PHI axis

Torque limited free rotation
 ± 0.2 deg.

OMEGA Translation
(crystal alignment)

**OMEGA XY
Centring table**
(Crystal centring)

Collision Detection
with Omega Stop safety switch

SmartMagnet
+ Holds the sample
+ Detects the sample

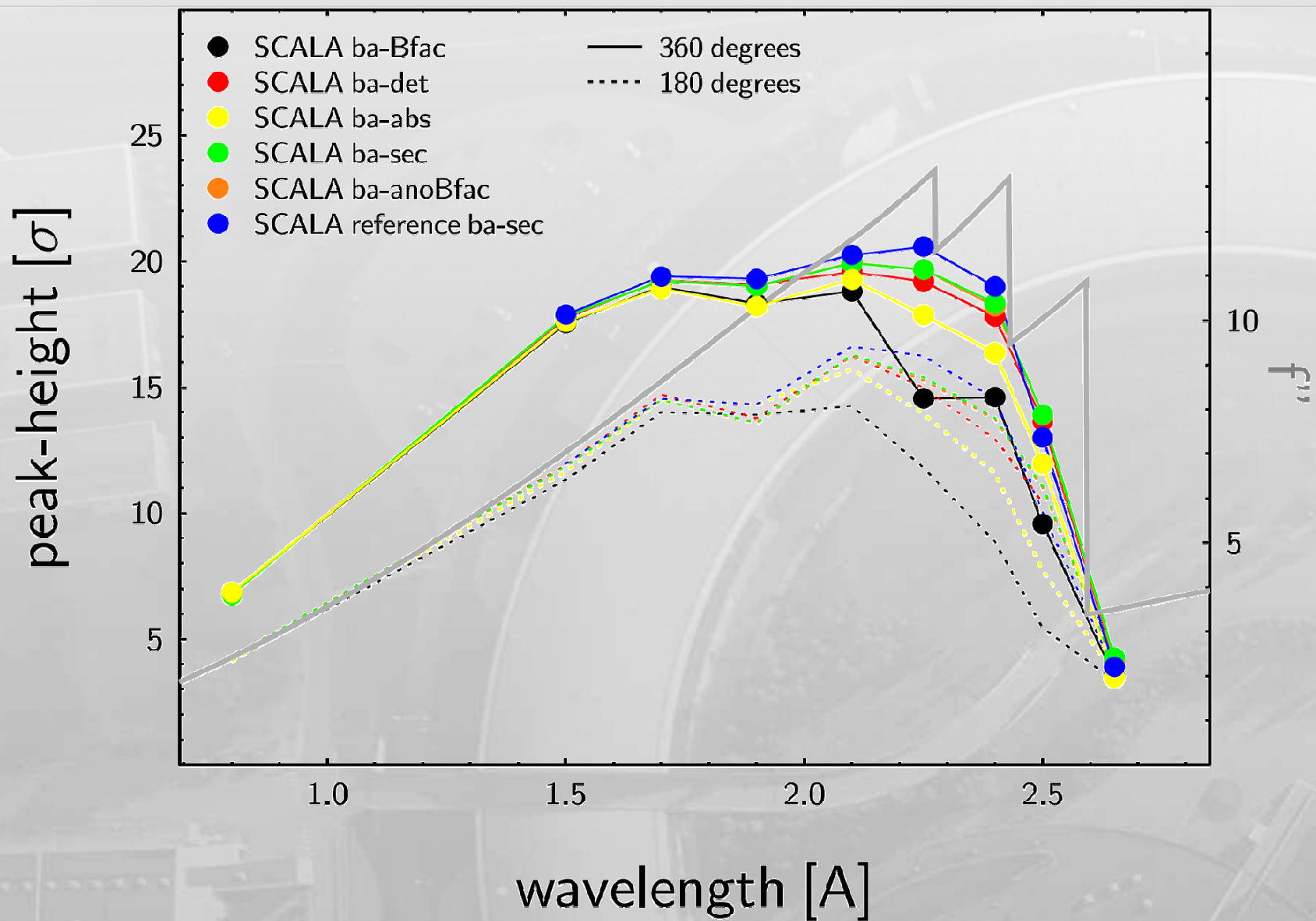
**SPINE
Sample holder**

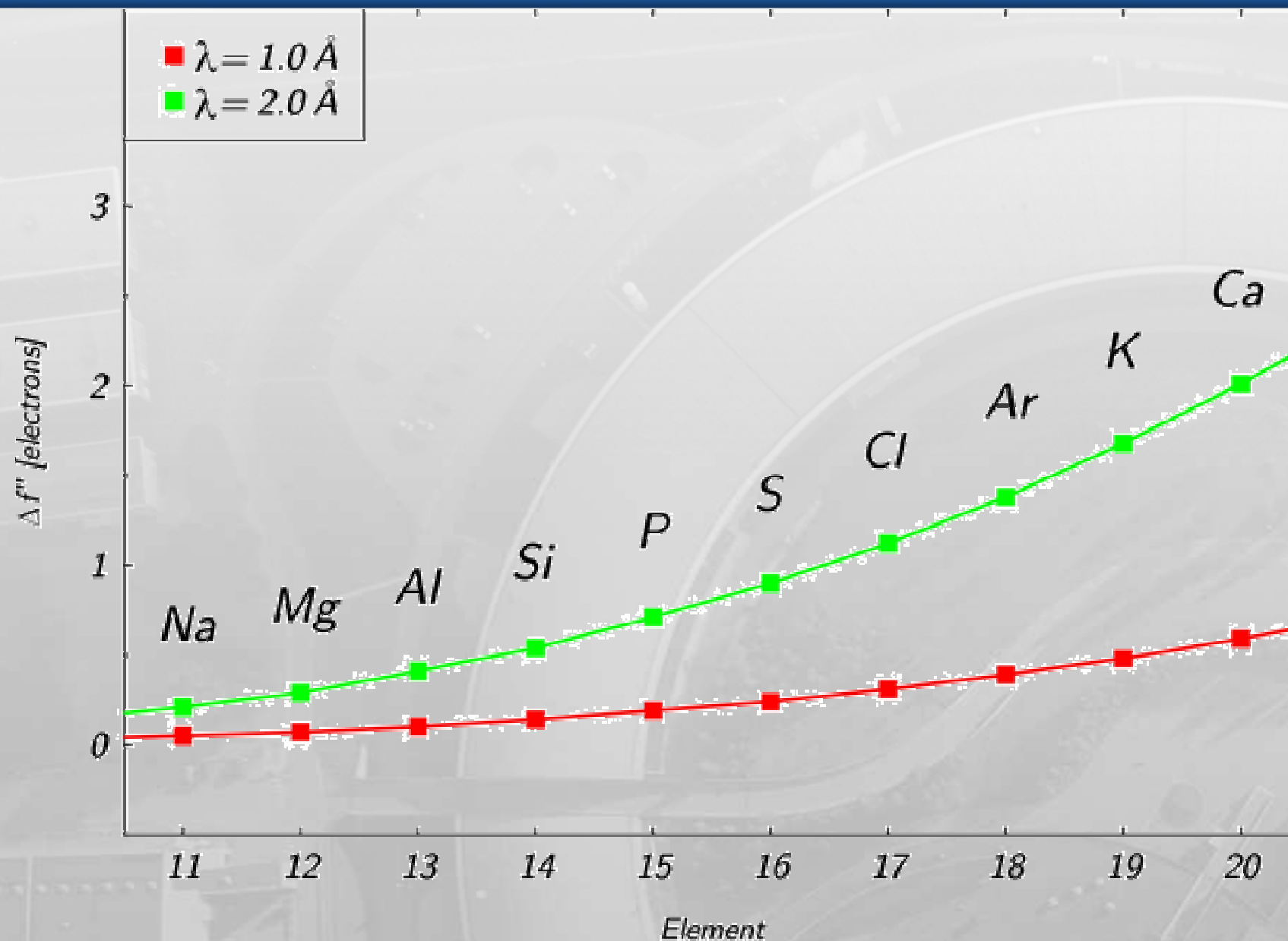
24 Deg

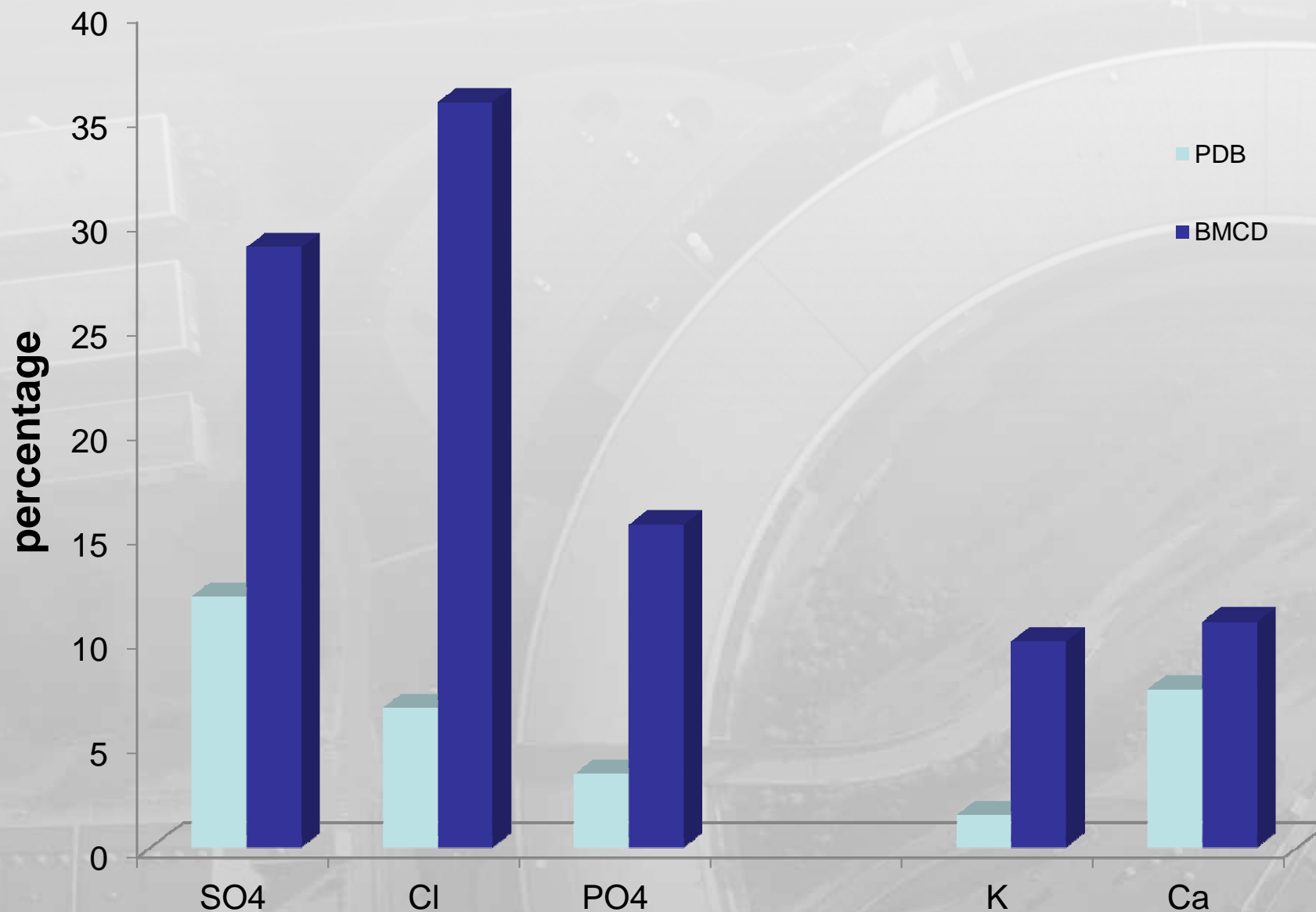
X-ray

EMBL Grenoble, F.Cipriani, S. Brockhauser, R. Ravelli

- Accurate data collection / processing
- If phasing: high redundancy / multiplicity
thorough scaling





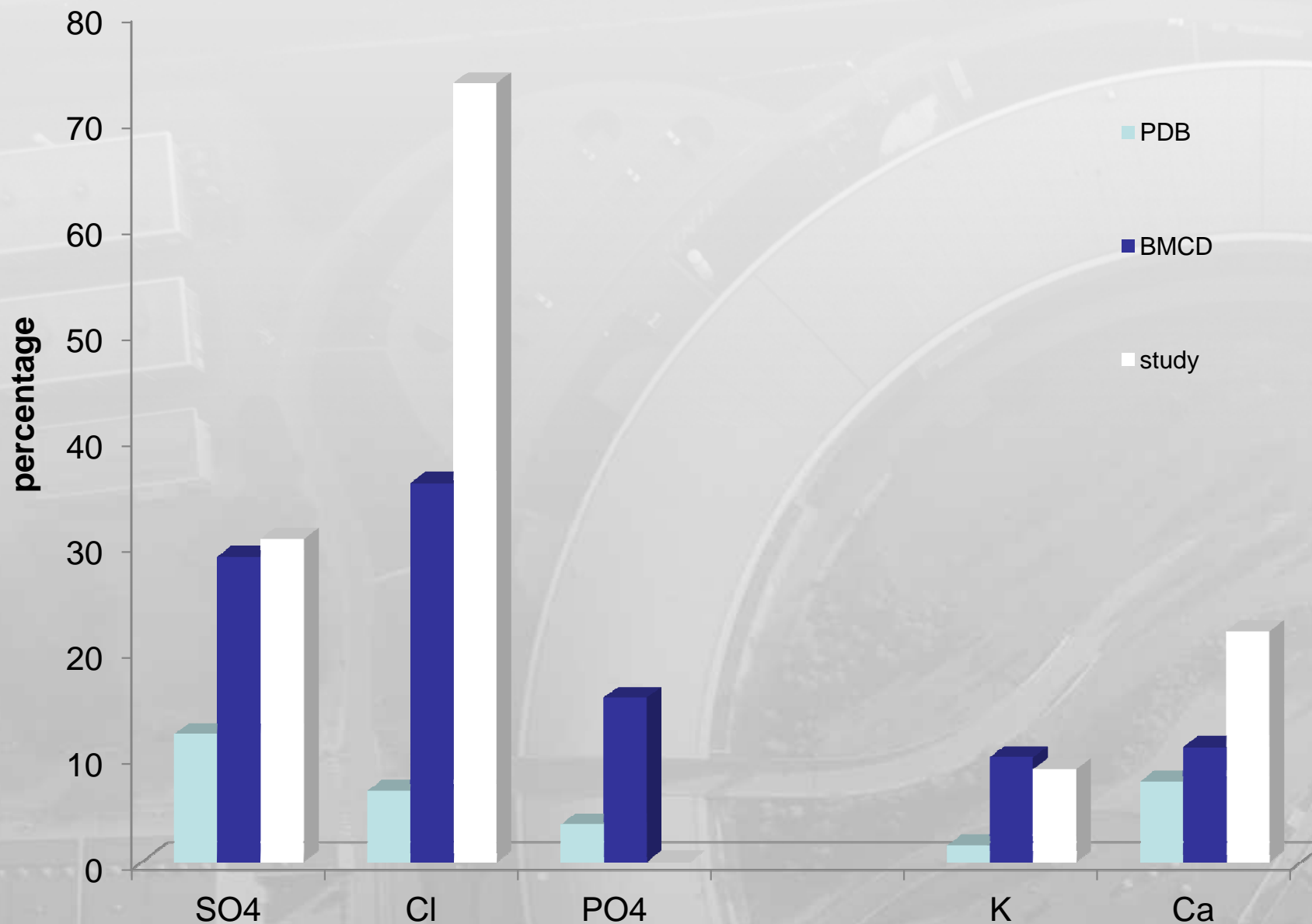


02/2012

protein	spacegroup	max. resolution [Å]	substructure	PDB code
apoferritin	F432	2.00	5 S; 2 Cl ⁻ 9(3) Cd ²⁺	2g4h
concanavalin A	I222	2.40	2 S; 1 Mn ²⁺ 1 Ca ²⁺ ; 1 Na ⁺ 3 Cl ⁻	2g4i
glucose-isomerase	I222	1.85	8 S; 1 Mg ²⁺ 1 Ca ²⁺ ; 1 Cl ⁻	2g4j
ADP-ribose hydrolase-3	P2 ₁ 2 ₁ 2 ₁	1.82	15 S; 2 Mg ²⁺ ; 2 Cl ⁻	2g4k
HEWL-pH4.5	P4 ₃ 2 ₁ 2	1.84	10 S; 7 Cl ⁻	2g4p
HEWL-pH8.0	P4 ₃ 2 ₁ 2	1.84	10 S; 5(4) Cl ⁻	2g4p
hydroxynitrile lyase	C222 ₁	1.84	6 S; 5(3) SO ₄ ²⁻ ; 1 Cl ⁻	2g4l
insulin	I2 ₁ 3	1.80	6 S	2g4m
α-lactalbumin	P2 ₁ 2 ₁ 2	2.30	42(54) S 6 Ca ²⁺ ; 2 K ⁺	2g4n
3-isopropylmalate dehydrogenase	P2 ₁ 2 ₁ 2 ₁	2.00	22(24) [†] S 2 SO ₄ ²⁻ ; 6 Cl ⁻	2g4o
moybdopterin-binding domain	P2 ₁	1.92	6 S; 1 Cl ⁻	2g4r

[†] 2 N-terminal Met residues missing. ^{††} missing S atom can be seen at 3.7σ.

protein	spacegroup	max. resolution [Å]	substructure	PDB-code
NBR1 PB1 domain	P6 ₃ 22	2.15	4 S; 1 Cl ⁻	2g4s
pancreatic elastase-Na	P2 ₁ 2 ₁ 2 ₁	2.15	10 S; 2 SO ₄ ²⁻ 1 Na ⁺	2g4t
pancreatic elastase-Ca	P2 ₁ 2 ₁ 2 ₁	1.84	10 S; 1 Ca ²⁺	2g4u
proteinase K	P4 ₃ 2 ₁ 2	2.14	10 S; 2 Ca ²⁺ 2 K ⁺ ; 1 Cl ⁻	2g4v
ribonuclease A	C2	1.84	23(24) ^{††} S 1 SO ₄ ²⁻ ; 1 Cl ⁻	2g4w
ribonuclease A	P3 ₂ 21	1.95	12 S; 1 SO ₄ ²⁻ 5 Cl ⁻	2g4x
thaumatin	P4 ₁ 2 ₁ 2	1.98	17 S	2g4y
thermolysin	P6 ₁ 22	1.98	2 S; 1 Zn ²⁺ 3(4) Ca ²⁺ 1 SO ₄ ²⁻ ; 8 Cl ⁻	2g4z
titin fragment		2.20	4 S; 2 Cl ⁻	2ill
trypsin	P1	1.84	7 S; 3 Cl ⁻ 0(3) SO ₄ ²⁻	2g51
trypsin	P2 ₁	1.84	7 S; 2 SO ₄ ²⁻	2g52
trypsin	P3 ₁ 21	1.82	14 S; 1 Ca ²⁺ 3 Cl ⁻	2g55



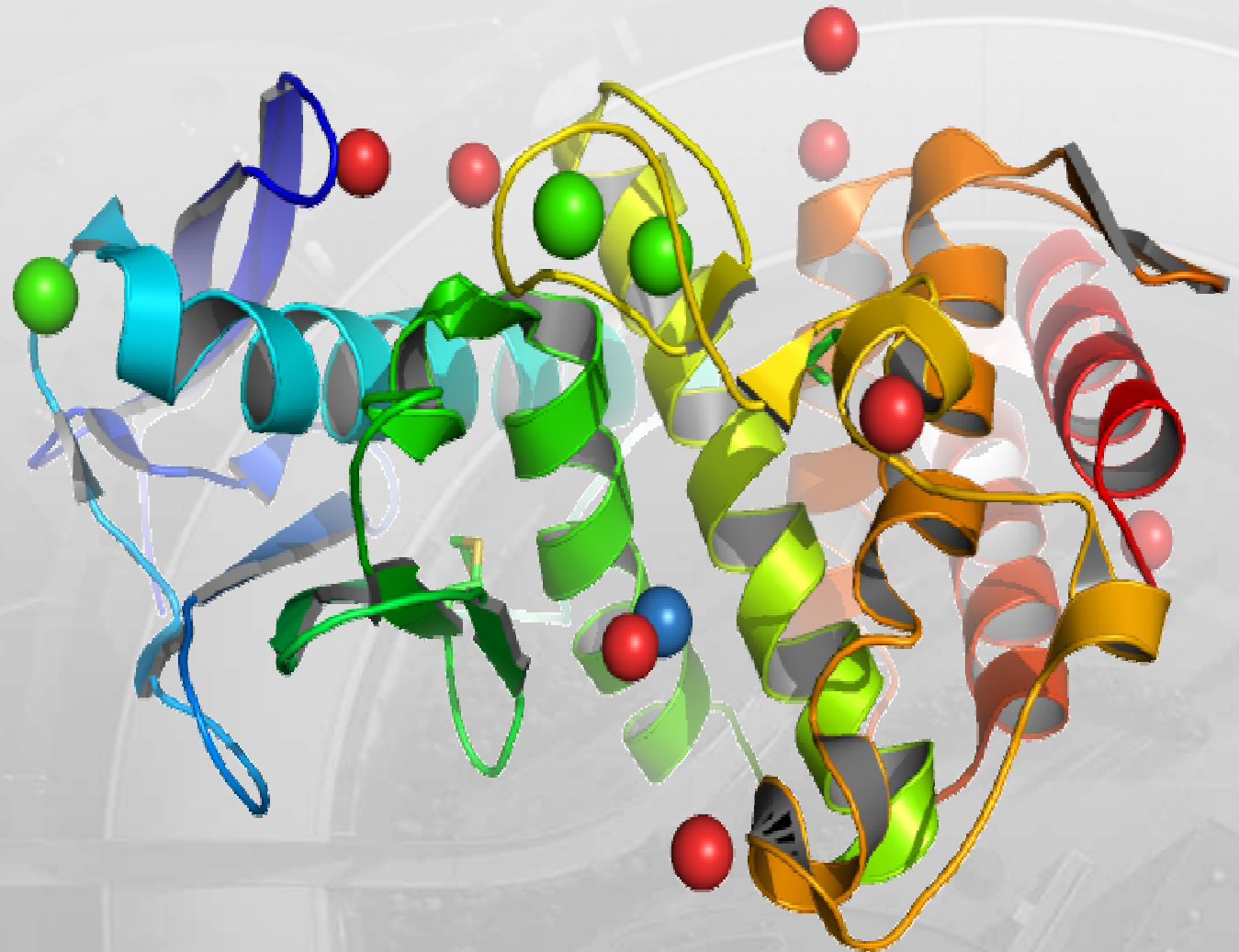
Thermolysin

1 Zn²⁺

3 Ca²⁺

8 Cl⁻

2 Met



Hydroxynitrile
lyase

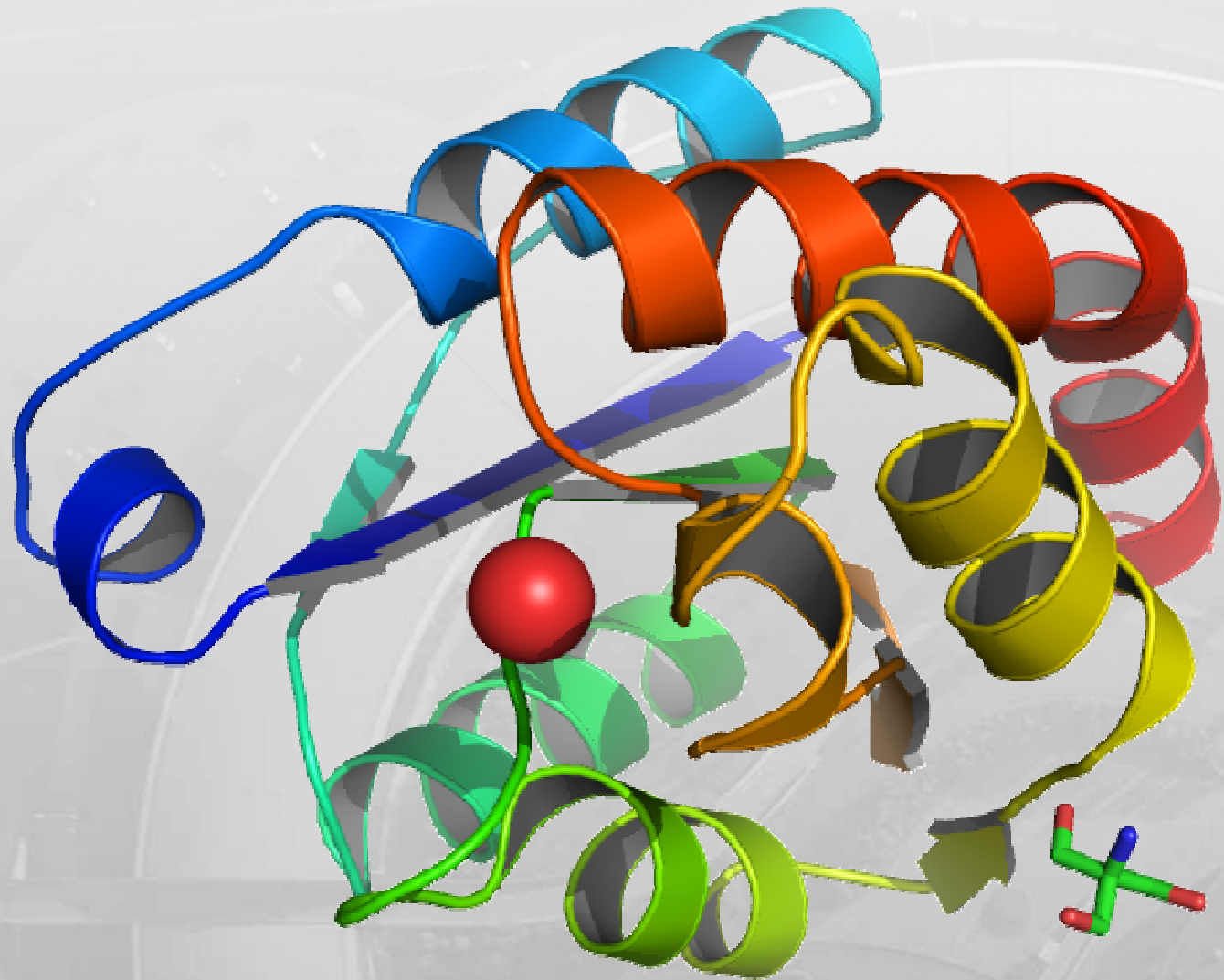
5 SO_4^{2-}
1 Cl^-

6 S
(alt. pos. +
HEC)

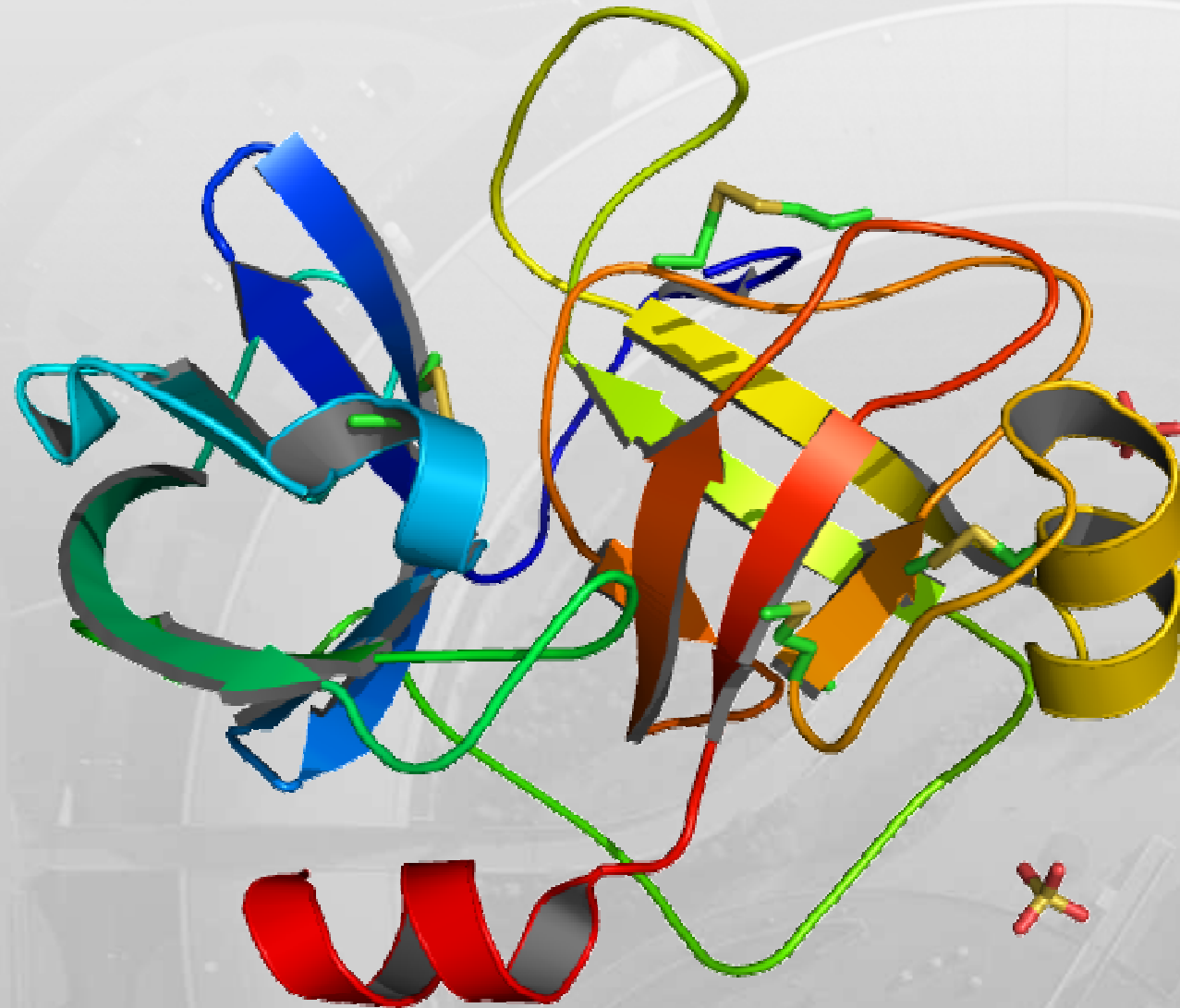


Molybdopterin
binding
domain (MogA)

Cl⁻ ion binds in
presumed PO₄³⁻
binding site

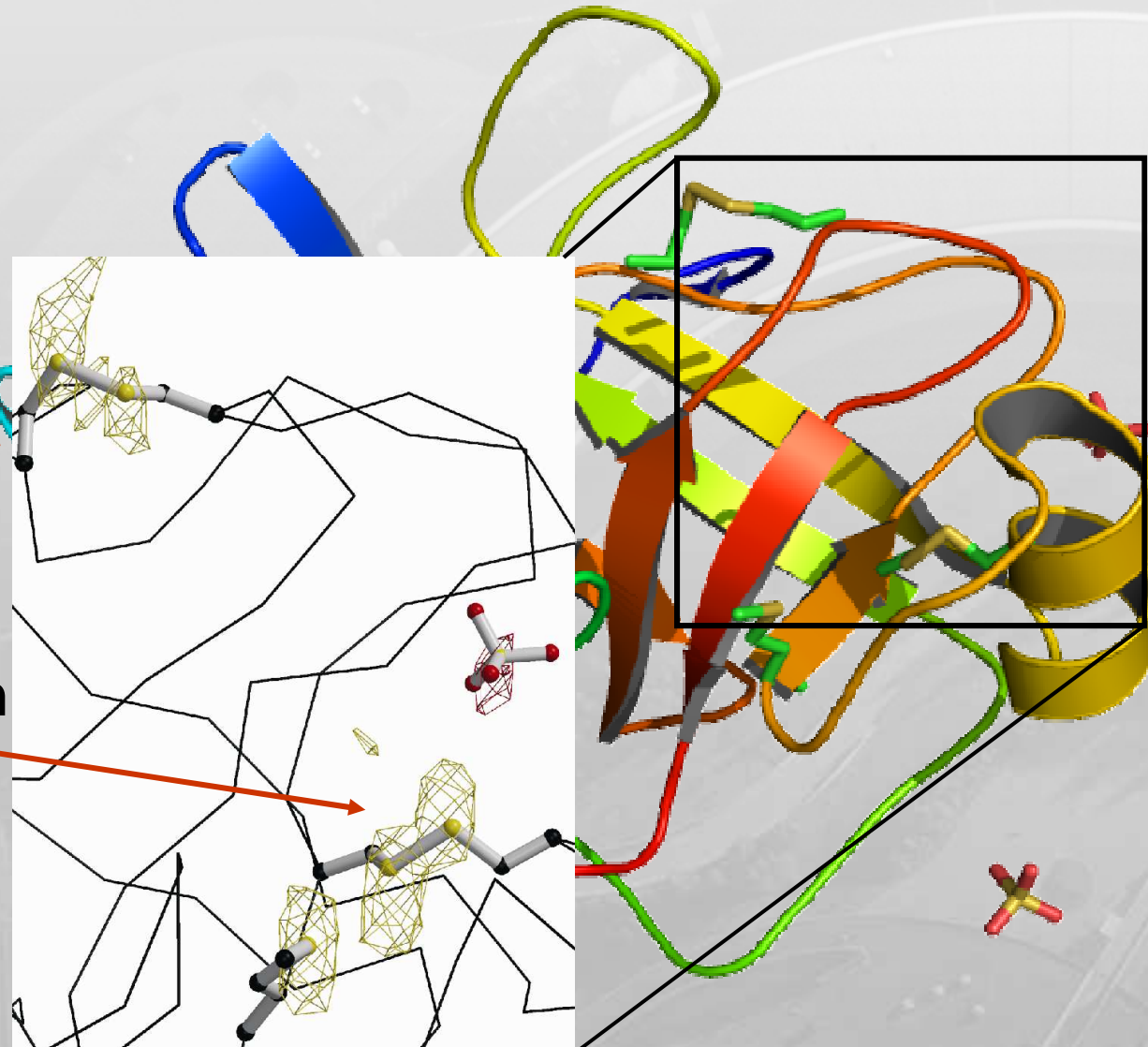


Trypsin



Trypsin

partial reduction
of SS-bridges



- only 2 out of 23 structures consist of S atoms only

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 - practically all protein S-atoms are visible
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- **high degree of reliability**
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BUT weakly bound ions with occupancies > 0.25 are uncertain.

- Collect accurate data !

S. Russi

